

Final Report

**Guidelines for Numerical Modeling
in Tier 3 Assessments and Other
Corrective Actions**

Submitted to:

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IOWA COMPREHENSIVE PETROLEUM UNDERGROUND STORAGE TANK FUND BOARD

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EXECUTIVE SUMMARY

Responsible parties have the option of using sophisticated computer models of groundwater at RBCA Tier 3 to assess in detail leaking underground storage tank sites that have been determined to be high risk after Tier 2 assessment. Engineers and geoscientists might also resort to such models in the design of a remediation system. Because of the wide range of possible Tier 3 approaches, there is no section of rules in the Iowa Administrative Code setting out Tier 3 modeling procedures. The rules do require that any such modeling must be shown to be valid before IDNR will approve a work plan or accept a Tier 3 report. This document aims to provide guidance for consultants who contemplate using a numerical modeling program such as Visual MODFLOW or GMS. The guidance stresses how one should approach a modeling project and how to report the results. The need to include in a report all details of the multi-step modeling process is treated. Three examples of numerical modeling of petroleum releases are provided from the western Iowa towns of Climbing Hill, Ida Grove, and Sioux City. The examples are not complete modeling reports of the type described in the text, but are included to show the degree of detail needed to accomplish such a project and to demonstrate validity to IDNR.

I. INTRODUCTION

When environmental risk at a leaking petroleum underground storage tank (LUST) site is characterized as high after a Tier 2 assessment, one of the options available for proceeding with obligatory corrective action is to do more realistic modeling of the site at Tier 3 to determine whether the over-simplifications inherent in the Tier 2 model are causing a false high risk condition. Modeling at Tier 3 can thus involve collecting site-specific information for various contaminant fate and transport parameters and employing this new information in numerical or analytical models that are more sophisticated than the one-dimensional analytical model in the IDNR software mandated for Tier 2 assessment. (567 IAC 135, section 11.2).

Modeling assessments at Tier 3 are advantageous for site owners and operators in situations where expensive corrective action would be required based on Tier 2 results, and where the Tier 2 model with default values for fate and transport parameters (567 IAC 135 Appx. A & B) does not reasonably reflect the hydrogeological conditions. Clearly, there will be significant expense in gathering additional site information. New monitor wells will likely be needed, with sophisticated soil and groundwater sampling to determine parameters such as soil-water partition coefficient and biodegradation rate constant. Additionally, for numerical or computer modeling of the groundwater and contaminant movement, much professional time will be required in information gathering, model set-up, model calibration, and report preparation. So the owner or operator of a LUST site, together with their certified groundwater professional, must balance the expense of Tier 3 modeling against other corrective action options. If the situation appears to justify a Tier 3 modeling approach, the groundwater professional has a range of models from which to choose. The report by Zhang et al. (2001) evaluates various

groundwater models or computer packages for Tier-3 numerical modeling and the groundwater professional is referred to that document for selecting modeling software. The current report provides guidelines for the groundwater professional on how to model a LUST site with any computer modeling software. Protocol for a Tier 3 modeling project is detailed and the outline of a modeling report is presented. Three examples of numerical modeling, arranged in order of increasing complexity, are provided. Examples in this report were done with the GMS software version 3.1 (Brigham Young Univ. EMRL. 2000). Guidelines for site assessment procedures at Tier 3 are available from IDNR (Lovanh *et al.*, 2000).

In this report, it is assumed that the groundwater professional has evaluated all feasible options for corrective action after the site of interest failed Tier 2 pathways, and has determined that building and calibrating a numerical model of the site is a necessary step toward obtaining eventual No Action Required status. In essence, this means that the groundwater professional thinks that numerical modeling is the most cost-effective way to demonstrate plume behavior or predict the efficacy of a particular active or passive corrective action.

The example models presented were developed from real LUST situations in western Iowa. The reader is cautioned, however, against basing any decisions concerning the sites on these modeling results. These models were prepared primarily as examples for this report, and are not guaranteed by the authors to be complete for all purposes.

II. NUMERICAL MODELING PROTOCOL

There are a number of steps involved in a numerical modeling project. The following is a modeling protocol with explanations for each of the steps involved. Additional discussion of these steps and a broader perspective on the philosophy of numerical modeling is found in Anderson and Woessner (1992).

Step 1: Purpose Establishment The first step in a modeling project, whether it be a Tier 3 assessment involving numerical modeling, or a passive natural attenuation design for a petroleum release, is to establish the purpose of using a groundwater model. Prior to proposing a modeling effort, a groundwater professional must have a clear understanding, in consultation with his or her client, the IDNR, and the ICPUST Fund Administrator, of what is needed at a site to obtain, for example, a “No Action Required” (NAR) designation, or to demonstrate that no high risk condition exists, or to demonstrate that natural attenuation is a viable corrective action alternative. A model can be used, for example, to show what effect a new pumping well might have on a nearby benzene plume, or what effect turning-off an existing water well might have on plume migration, or how source removal might enhance plume degradation.

Step 2: Hydrogeological Characterization Proper characterization of the hydrogeological conditions at a site is necessary in order to understand the importance of relevant flow or solute transport processes. With the increase in the attempted application of intrinsic remediation as a remedial action, it is imperative that a thorough site characterization be completed. This level on characterization requires more field work, including more monitoring wells, groundwater samples, and an increase in the number of laboratory analyses to determine important field parameters. Without proper site characterization, it is not possible to select an

appropriate model or develop a reliably calibrated model. The following hydrogeological and geochemical information must be available for this characterization:

- Regional geologic data depicting subsurface geology.
- Topographic data (including surface-water elevations).
- Stream-discharge (base flow) data (if water budgets are of interest).
- Well construction diagrams and soil boring logs.
- Geologic cross-sections drawn from soil borings and well logs.
- Measured hydraulic-head data for several years.
- Estimates of hydraulic conductivity derived from aquifer and/or slug test data.
- Location and estimated flow rate of groundwater sources and sinks.
- Identification of chemicals of concern in contaminant plume.*
- Vertical and horizontal extent of contaminant plume.*
- Location, history and mass loading or removal rate for contaminant sources or sinks.*
- Direction and rate of contaminant migration.*
- Identification of downgradient receptors. *
- Partition coefficient (K_d) or organic carbon content of sediments.*
- Appropriate geochemical field parameters (e.g. dissolved oxygen, other electron acceptors, Eh, pH, degradation byproducts)*

(Those marked with ‘*’ are required for certain fate and transport models.) This information should be presented in maps, tables or graphs in a report documenting model development.

Step 3: Model Conceptualization Model conceptualization is the process in which data describing field conditions are assembled in a systematic way to demonstrate groundwater flow and contaminant transport processes at a site. The model conceptualization aids in determining both the modeling approach and which model software to use. Questions to ask in developing a conceptual model include, but are not limited to:

- Are there adequate hydrogeological data to describe the conditions at the site?
- In what direction is groundwater moving?
- Can the groundwater flow or contaminant transport be characterized as one-, two- or three-dimensional?
- Is the hydrogeologic system composed of more than one aquifer, is vertical flow between aquifers important?
- How does recharge to the aquifer occur: by precipitation, or by leakage from a river, drain, lake, or infiltration pond, or a combination of these?
- Is groundwater leaving the aquifer by seepage to a river or lake, flow to a drain, or extraction by a well? Is evapo-transpiration important?

- Does it appear that the aquifer hydrogeological characteristics remain relatively uniform, or do geologic data show significant variation over the site?
- Have the boundary conditions been defined around the perimeter of the model domain, and do they have a hydrogeological or geochemical basis?
- Do groundwater flow or contaminant source conditions remain constant, or do they change with time?
- Are there receptors located generally down-gradient of the contaminant plume?
- Are the geochemical processes taking place in onsite groundwater fully known?

Other questions related to site-specific conditions may be asked. This conceptualization step must be completed and described in the model documentation report.

Step 4: Model Design In the model design all parameters needed to run a model are set, this step should emphasize the rationale for modeled parameter values. Listing of all variations of a parameter throughout the model is not necessary. Data gaps, anomalies, or uncertainties should be discussed. The input parameters include the following for each model layer:

- Model grid size and spacing
- Layer elevations
- Boundary conditions
- Hydraulic Conductivity/Transmissivity
- Recharge
- Transient or steady state modeling
- Dispersion coefficients
- Degradation rate and sorption coefficients; porosity and bulk density.

Step 5: Model Calibration Model calibration consists of changing values of model input parameters in an attempt to match field conditions within some acceptable criteria. The calibration process applies to both steady-state and transient simulations. With steady-state simulations, there are no observed changes in hydraulic head or contaminant concentration with time for the field conditions being modeled. Transient simulations involve the change in hydraulic head with time (e.g. aquifer test or an aquifer stressed by a well field). Transient models may be calibrated without simulating steady-state flow conditions, but this involves

additional complexity. Data describing field conditions may consist of measured hydraulic heads, groundwater or streamflow rates, or contaminant plume migration rates. Model calibration requires that field conditions at a site be properly characterized. Lack of proper site characterization may result in a model calibrated to a set of conditions that are not representative of actual field conditions.

At a minimum, for LUST sites, comparisons should be made between model-simulated conditions and field conditions for the following data:

- Hydraulic head data
- Groundwater-flow direction
- Hydraulic-head gradients
- Contaminant migration rates
- Contaminant migration directions
- Contaminant concentrations

These comparisons should be presented in maps, tables, or graphs. Each modeler and model reviewer will need to use their professional judgment in evaluating the calibration results. For initial assessments, it is possible to obtain useful results from models that are not calibrated. The application of uncalibrated models can be very useful as a screening tool or in guiding data collection activities.

Calibration is typically characterized for matching the modeled hydraulic head and contaminant concentrations with observed ones. There are no universally accepted "goodness-of-fit" criteria that apply in all cases. However, it is important that the modeler make every attempt to minimize the difference between model- simulated and field conditions. A reasonably good calibration for the head at a particular monitor well might be within one foot of observed head, with a RMS (root-mean-square) error of 5%. For the contaminant parameter, good calibration might be modeled benzene concentration at the well within 500 ug/L of latest observed sample results.

Another parameter that can be calibrated is the water budget. This is a balance sheet of the amount of water entering and leaving a modeled system. For fate and transport models of LUST sites, calibration of a water budget for the flow domain is generally not necessary. Such an effort would require quantitative knowledge of recharge, and of water movement at all domain and layer boundaries and would require an extensive observation well network and instrumentation of any streams in the domain. It is enough for most LUST site modeling to demonstrate (through calibration) that hydraulic heads, flow directions and gradients, and contaminant concentrations around the site of interest match real site observations.

Step 6: Sensitivity Analysis A sensitivity analysis is the process of varying certain poorly constrained model input parameters over a reasonable range (range of uncertainty in value of model parameter) and observing the relative change in model response. Typically, the observed change in hydraulic head, flow rate or contaminant transport are noted. The purpose of the sensitivity analysis is to demonstrate the sensitivity of the model simulations to uncertainty in values of model input data. The sensitivity of one model parameter versus other parameters is also demonstrated. Sensitivity analyses are also beneficial in determining the direction of future data collection activities. Data for which the model is relatively sensitive would require future characterization, as opposed to data for which the model is relatively insensitive. These data would not require further field characterization.

Step 7: Predictive Simulations A model may be used to predict some future groundwater flow or contaminant transport condition. The model may also be used to evaluate different remediation alternatives, such as hydraulic containment, pump-and-treat or intrinsic remediation and to assist with risk assessment. In order to perform these tasks, the model, whether it is a groundwater flow or solute transport model, must be reasonably accurate, as

demonstrated during the model calibration process. However, errors and uncertainties in a groundwater flow analysis and solute transport analysis make any model prediction no better than an approximation. For this reason, all model predictions should be expressed as a range of possible outcomes that reflect the uncertainty in model parameter values.

Step 8: Performance Monitoring Plan Groundwater models are commonly used to predict the hydraulic performance of a groundwater system or the migration pathway and concentrations of contaminants in groundwater. The accuracy of model predictions depends upon the degree of successful calibration of the model in determining transport flow directions or chemical reactions, and the applicability of the groundwater flow and solute transport equations to the problem being simulated. Errors in the predictive model, even though small, can result in gross errors in solutions projected forward in time. Performance monitoring is required to compare future field conditions with model predictions.

The degree of monitoring needed to compare future field conditions with model predictions depends on the level of confidence in the model results and the associated level of risk to the downgradient receptors. The length of the performance-monitoring period should be based, in part, on model predictions, but more importantly on actual laboratory analytical data, trends in analytical data from the sampling events, and on professional judgement.

The performance-monitoring plan should include proposed well locations, screen locations, pumping rates, etc. A monitoring plan should be part of most reports because any predictions must be viewed as estimates, dependent upon the quality and uncertainty of the input data. The physical processes governing groundwater flow, solute transport and parameters used as model input can only be approximated. Models may be used as predictive tools, however field monitoring must be incorporated to verify model predictions.

III. NUMERICAL MODELING REPORT

A numerical modeling report details a groundwater model developed for a specific purpose, for a specific LUST site. Each of the steps in the modeling process should be described in sufficient detail so that the model reviewer may determine the appropriateness of the model for the site or problem that is simulated. The report must include the following information:

- A description of the purpose of the model application.
- Presentation of the hydrogeologic data used to characterize the site.
- Documentation of the source of all data used in the model, whether derived from published sources or measured or calculated from field or laboratory tests.
- Description of the conceptual model.
- Identification of the model package selected to perform the task, its applicability and limitations. A discussion of the modeling approach (steady-state vs transient; continuous source vs decaying source, etc.).
- Documentation of all calculations.
- Summary of all model calibration, history matching and sensitivity analysis results.
- All model predictive simulation results presented as a range of probable results given the range of uncertainty in values of model parameters.

The following sections should be included, as appropriate, in a modeling report. In some cases, additional information may be necessary to convey a complete understanding of the groundwater model.

- Title Page
- Table of Contents
- List of Figures
- List of Tables
- Executive Summary
- Introduction
- Objectives
- Hydrogeologic Characterization
- Groundwater Flow Modeling
 - Model Conceptualization and Design
 - Input parameters
 - Calibration
 - Sensitivity Analysis
 - Predictive Simulations

- Contaminant Transport Modeling
 - Model Conceptualization and Design
 - Input parameters
 - Calibration
 - Sensitivity Analysis
 - Predictive Simulations
- Performance-Monitoring Plan
- Summary and Conclusions
- References
- Well Data
- Additional Data

The tables and figures should be placed wherever they are needed to demonstrate clearly the author's purposes. The following is a list of tables that should appear within the body of the model documentation report or in attached appendices:

- Well and boring log data including:
 - Well name
 - XY coordinate data in the model.
 - Top of casing.
 - Ground elevation.
 - Well screen interval and layer designation.
 - Piezometric elevation data.
 - Bottom of layer elevations.
 - Hydraulic conductivity/transmissivity.
 - Groundwater quality chemical analyses, if appropriate.
 - Aquifer test or slug test data.
- Model calibration result showing a comparison of measured and simulated calibration targets and residuals.
- Results of sensitivity analysis showing the range of adjustment of model parameters and resulting change in hydraulic heads or groundwater flow rates.
- Other data, not listed above, may lend itself to presentation in table format.

The following is a list of the types of figures (maps or cross sections) that should be included in the model documentation report:

- Regional location map with topography.
- Site map showing soil boring and well locations, and site topography.
- Geologic cross sections.
- Map showing the measured hydraulic-head distribution.
- Maps of top and/or bottom elevations of aquifers and confining units.

- Areal distribution of hydraulic conductivity/transmissivity.
- Map of areal recharge (if appropriate).
- Simulated hydraulic-head maps.
- Contaminant distribution map(s) and/or cross sections showing vertical distribution of contaminants (if appropriate).
- Map showing simulated contaminant plume distribution (if appropriate).

Other types of information, not listed above, may be presented in graphic format. Figures that are used to illustrate derived or interpreted surfaces such as layer bottom elevations and hydraulic-head maps should have the data used for the interpolation also posted upon the figure.

IV. NUMERICAL MODELING EXAMPLES

Three sites, Climbing Hill, Ida Grove, and Cook Park, are simulated as examples. All three sites are located in the west of Iowa (Figure 1). Modeling complexity is simplest at Climbing Hill and most complicated at Cook Park. The examples given are not in the complete format for a modeling report as outlined above, but are provided to show the basic elements of modeling objectives, site characterization, and model design are used to build LUST site models, and show the degree of detail involved in model reporting. The conceptual approach in GMS v.3.1 was used for the modeling task. This software was selected after evaluating several computer software packages for RBCA Tier-3 assessment (Zhang, et al., 2001). All models are steady-state simulations of groundwater flow onto which a transient simulation of contaminant transport is conducted. In all examples the meter or foot is the unit of length, day is the unit of time, and ug/L is the unit of contaminant concentration.

Coordinates are given for features in the models in some of the tables. There are two coordinate systems in each model, one is an X-Y system in meters, based on a world map, the other is an I-J-K index system for individual cells of the three-dimensional model grid created in MODFLOW and MT3DMS. The world coordinates for the modeled locations were obtained with the help of Mary Howes and Paul Liu of the Iowa Geological Survey Bureau. For the model cells, the I-J origin is at the upper left of the grid, and the layer is denoted by K.

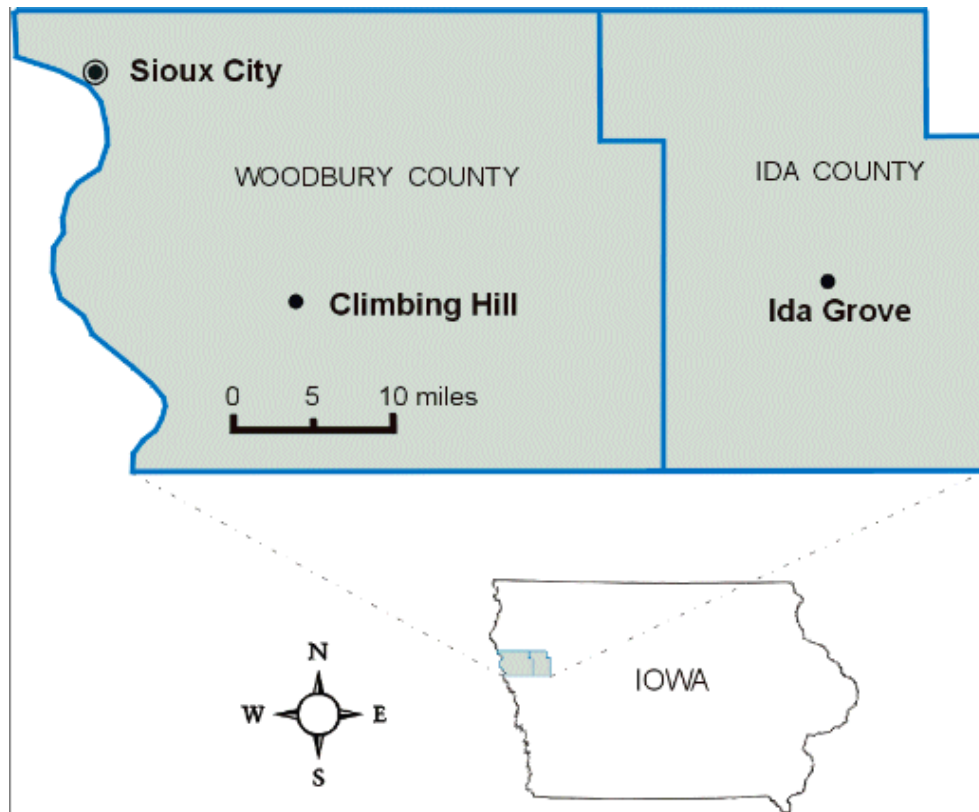


Figure 1 Locations of the three sites in Iowa

A. Climbing Hill

A.1 Statement of Problem

The town of Climbing Hill is located in central Woodbury County, on the lower slope of an upland that rises east of the West Fork of the Little Sioux River. The town has some small, private water supply wells that produce from thin, sandy layers at depths of about 75 ft. The producing zone is stratigraphically at the contact between Pre-Illinoian till and overlying loess. Other wells go into a sandstone layer beneath a shale layer in the Cretaceous Age Dakota Formation (Fm.) that directly underlies the Pre-Illinoian till. Petroleum contamination has

shown up in several of the water wells screened in the shallower sandy interval; petroleum contamination has not been found in water wells screened in the Dakota Fm.

A.2 Objectives

The purpose of modeling groundwater flow and contaminant transport at Climbing Hill was to determine

- 1) what the regional flow in the area is;
- 2) what effect the residential wells have on the flow;
- 3) what forms a benzene plume and a TEH plume, the latter is simulated as xylene and can be expected to have in the two-layer aquifer.

A.3 Hydrogeologic Characterization

Maps, borehole logs, water level data, other hydrogeological information, and groundwater contaminant concentrations for Climbing Hill are taken from the IDNR LUST files #7LTV89 and 8LTU14. The latter file includes a report entitled “Feasibility Analysis Report” (EnecoTech, 1997) which contains information for several water wells in the town. The petroleum source is located along Woodbury Co. Rd. D-54, near the east end of town. The times and amounts of petroleum releases are uncertain.

According to the Geological Survey Bureau of IDNR, Climbing Hill is within the Loess Hills landform region and the near surface stratigraphy consists of thick loess overlying Pre-Illinoian glacial deposits; both sedimentary packages are of Pleistocene Age. Westward, toward the river, this stratigraphy is complicated by Holocene Age erosional processes and alluvial deposition in the floodplain and terraces. (Jean Prior, written communication, June, 2001).

There is no information available that provides good stratigraphic control of this lateral stratigraphic transition.

The water table is between 20 and 30 ft deep in the loess, and slopes westward. Annual recharge to the water table is not precisely known, but is likely in the range of 2 to 6 inches ($0.051 - 0.152$ m/y) or 7 – 25 % of annual precipitation. Existing monitor wells are completed in the loess; residential wells are completed in the sand layer underlying the loess.

A.4 Groundwater Flow Modeling

A.4.1 Conceptualization and Design

The simulation domain is a small groundwater basin (Figure A-1), which is bounded by a topographic high or groundwater divide in all directions except to the west. The west boundary is formed by the West Fork Little Sioux River that flows from north to south. The river elevation varies from 329.8 m to 328.4 m along the domain boundary. The river is assumed to be well connected to the aquifers and thus is modeled as constant-head boundary (the red crosses in Figure A-1). There are three unnamed creeks (Creeks 1, 2, and 3) inside the domain, which are modeled with the drain package in MODFLOW.

A three-dimensional, two-layer model was constructed to examine hydraulic behavior and contaminant transport at Climbing Hill. The first layer is for the loess and the second layer is for the thin, sandy layer used as a water source. Figure A-2 is a cross section of the conceptual model. Three wells screened in the thin sand layer are included in the model. These wells are intended to simulate residential water demand, and so are assigned small pumping rates of $18 \text{ m}^3/\text{d}$ (20 gpm for about 4 hrs/d). The wells are located in the grid (Table A-1) at points corresponding to water wells # 4, #6, and #11 in the EnecoTech (1997) document.

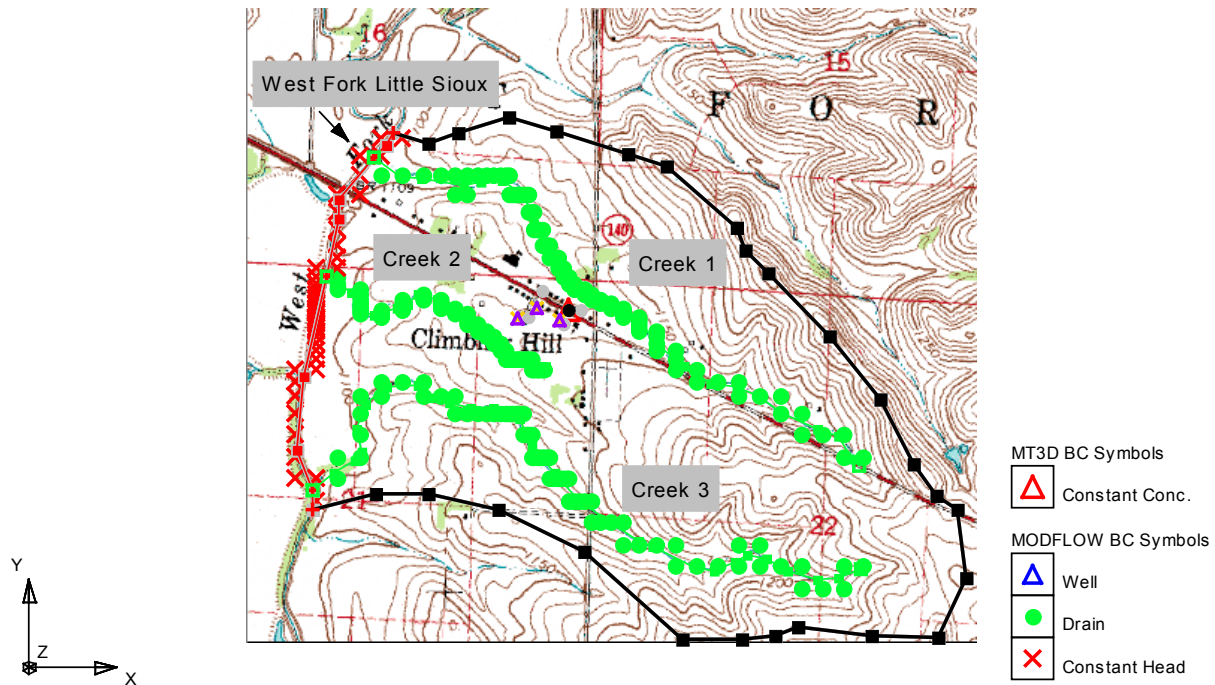


Figure A-1. The simulation domain with boundary conditions at Climbing Hill

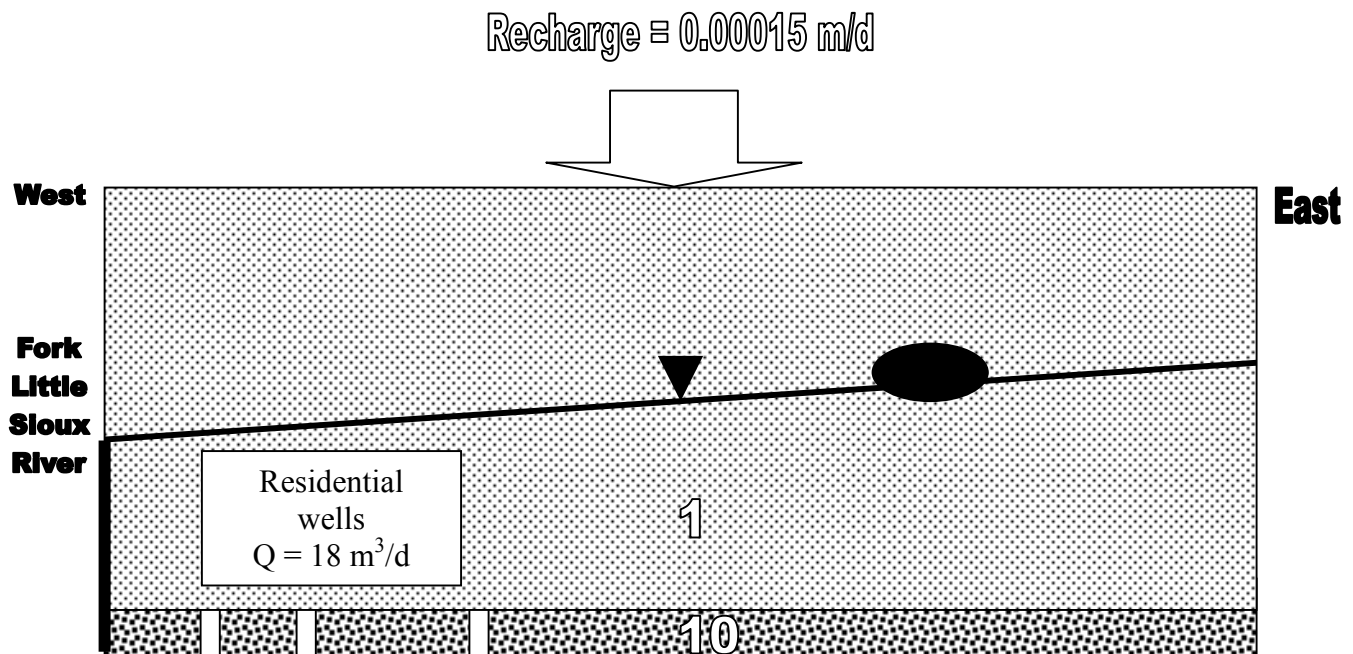


Figure A-2. Schematic E-W cross section of the Climbing Hill conceptual model. Not to scale. Black triangle denotes water table; black oval denotes petroleum source. Numbers within various fields are hydraulic conductivity (m/d) for the unit indicated.

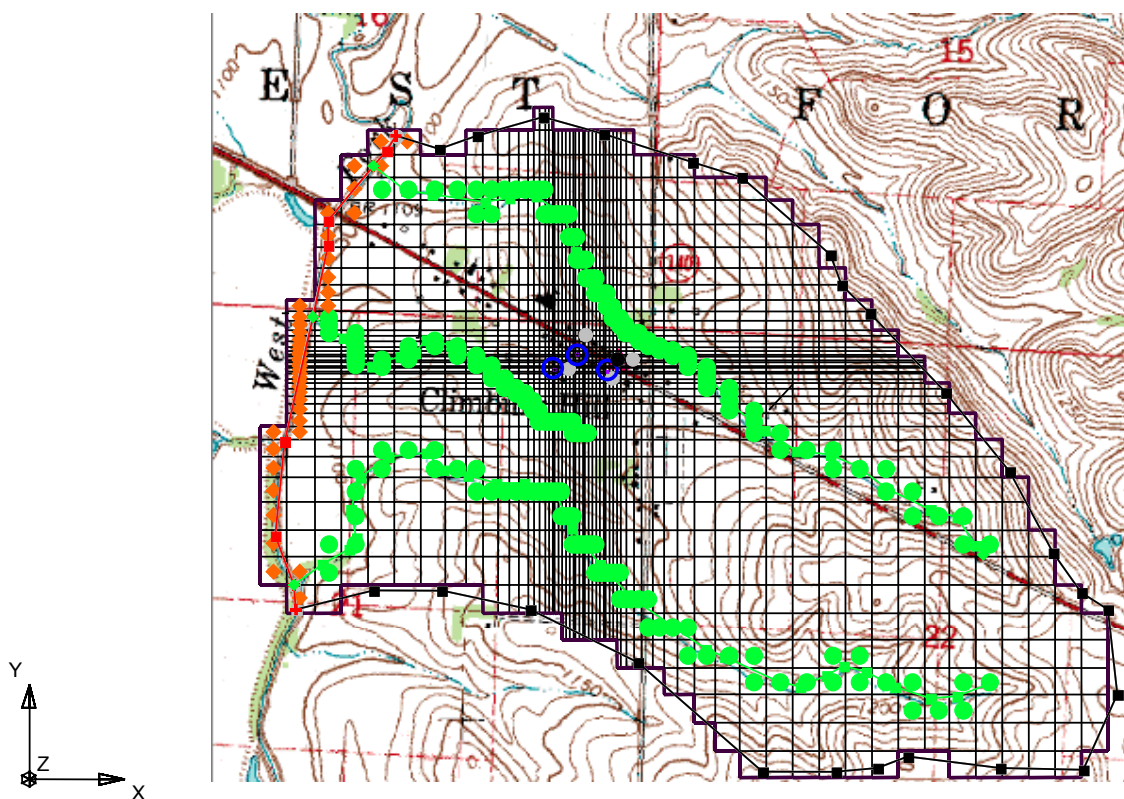


Figure A-3 Finite difference grids of the modeling domain at Climbing Hill

Table A-1. Parameters for grid refinement at the three wells

Well #	Refine grid in X direction			Refine grid in Y direction		
	Base cell size	Bias	Max cell size	Base cell size	Base	Max cell size
4	7.5	1.2	75	7.5	1.2	75
11	7.5	1.2	75	7.5	1.2	75
6	7.5	1.2	75	N/A	N/A	N/A

A.4.2 Input Parameters

Four coverages for the model domain, Source/Sink, Layer 1, Layer 2, and Recharge, were created in GMS. The packages used in MODFLOW are: Basic, BCF, Well, Drain, Recharge, PCG2, and Output Control. The West Fork Little Sioux River is simulated as a constant-head boundary and the three creeks are simulated with the drain package in MODFLOW. The river stage and the bottom elevation and conductance of the three creeks are listed in Table A-2. Table A-3 provides the locations and pumping rates for the three wells.

Table A-2. Input parameters for the river and creeks.

	W. Fork Little Sioux River	Creek 1	Creek 2	Creek 3
Simulated in MODFLOW by	Constant head	Drain	Drain	Drain
River stage (<i>m</i>)	328.4 - 329.8	N/A	N/A	N/A
River or drain bottom elevation (<i>m</i>)	N/A	329.7-371.8	329.2-347.5	328.4-374.9
River or drain conductance (m/day)	N/A	5.0	5.0	5.0

Table A-3 Pumping well locations and rates

Well #	X (<i>m</i>)	Y (<i>m</i>)	I	J	K	Pumping Rate (<i>m</i>³/<i>day</i>)
4	246282	4692159	19	27	2	-18
11	246218	4692121	24	20	2	-18
6	246365	4692116	25	36	2	-18

The loess is simulated with the coverage Layer 1. This layer is treated as an unconfined, horizontal aquifer with bottom elevation at 326.1 m. The thin sandy layer is modeled by the coverage Layer 2 with a uniform thickness of 2.1 m, and is also horizontal. Both layers are treated as homogeneous. The hydraulic conductivity for Layer 1 is one order of magnitude smaller than that of Layer 2 (Table A-4). Hydraulic conductivity is assumed to be isotropic, i.e., $K_h = K_v$.

Table A-4 Input parameters of the layers for groundwater flow modeling

	Layer 1	Layer 2
Aquifer Type	Unconfined	Confined
Top Elevation (<i>m</i>)	400	326.1
Bottom Elevation (<i>m</i>)	326.1	324.0
Horizontal Conductivity, K_h (<i>m/day</i>)	1.0	10
Vertical Conductivity, K_v (<i>m/day</i>)	1.0	10
Net Recharge Rate (<i>m/d</i>)	0.00015	N/A

A.4.3 Model Calibration

The flow model is calibrated against the long-term average of the observed hydraulic heads at eleven monitoring wells by changing the hydraulic conductivity, the net recharge rate, and the conductance of the creeks. The calibration target is set to be within 0.5 m of the observed water levels at eleven monitor wells, and the results are listed in Table A-5. All errors are much smaller than 0.5 m. The Root Mean Square Error is 0.19 m. The calibrated conductance values

are listed in Table A-2, the calibrated hydraulic conductivity values are listed in Table A-4, and the calibrated net recharge rate is 0.00015 m/d (2.1 in/yr). The calibrated steady-state head contours are illustrated in Figure A-4 along with a scatter plot and error summary of the observed versus modeled head at the four monitoring wells.

Table A-5 Calibration results for hydraulic heads at the observation wells

Well #	X (m)	Y (m)	I	J	K	Observed head (m)	Simulated head (m)	Error (m)
MW 7	246265	4692177	17	25	1	334.40	334.37	-0.03
MW 12	246302	4692217	14	29	1	334.40	334.66	0.26
MW 18	246396	4692151	20	39	1	335.50	335.28	-0.22
MW 101	246433	4692151	20	41	1	335.40	335.55	0.15
MW 103	246373	4692101	26	37	1	335.00	335.15	0.15
MW 105	246265	4692128	23	25	1	334.60	334.42	-0.18
MW 106	246348	4692179	17	31	1	335.00	334.94	-0.06
MW 112	246299	4692178	17	29	1	334.40	334.58	0.18
MW 113	246255	4692128	23	24	1	334.50	334.36	-0.14
MW 115	246396	4692136	22	39	1	335.60	335.29	-0.31
MW 118	246337	4692178	17	33	1	335.10	334.86	-0.24
Root Mean Square Error = 0.19								

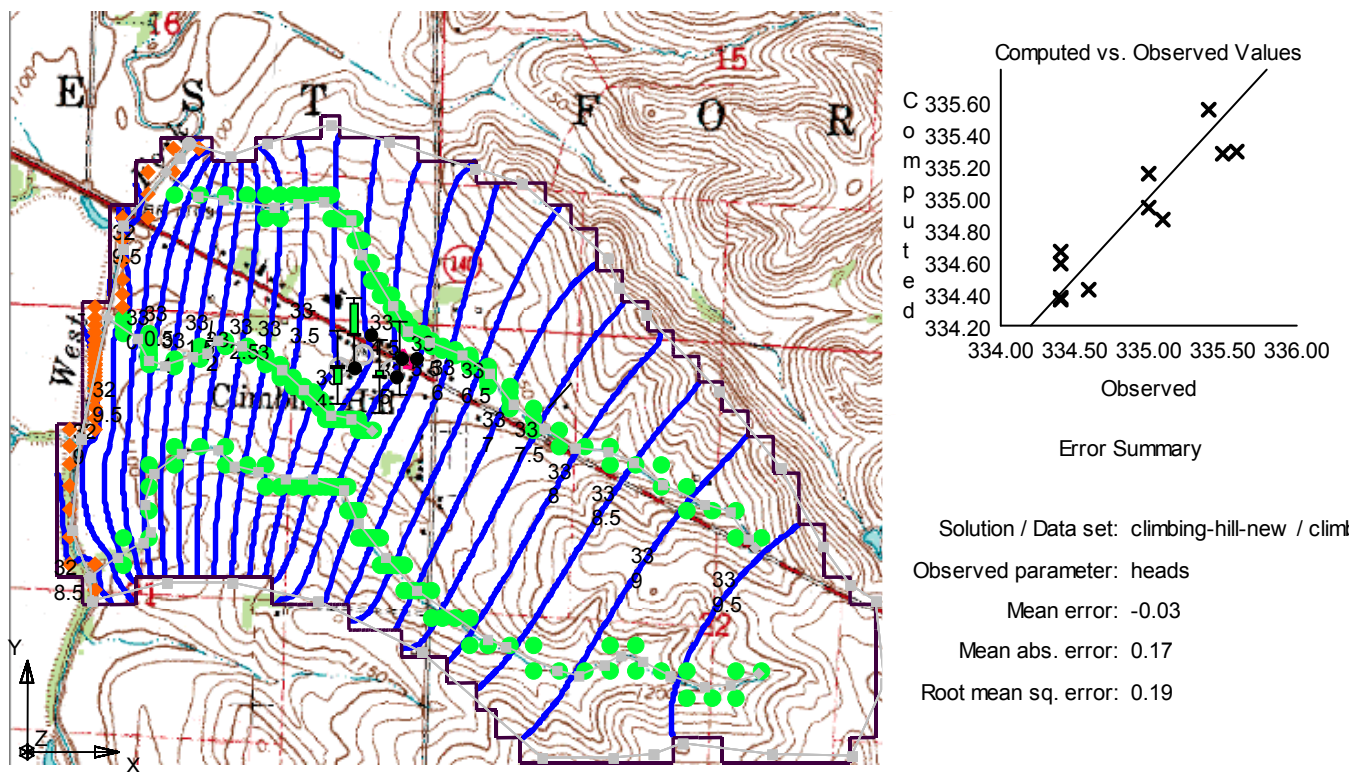


Figure A.4 Steady-state hydraulic head contours with calibration

A.4.4 Sensitivity Analysis

A sensitivity analyses for the Climbing Hill model was carried out by doubling the values of hydraulic conductivities and recharge rate. The simulation results are given in Table A-6, where it is seen that all modeled heads are higher than observed ones. This result is due to the dominance of the low permeability Layer 1 on effective hydraulic conductivity of the hydrostratigraphic sequence. The RMSE increased from 0.19 to 0.64 with the largest error of 0.88 m at MW-12.

Table A-6 Comparison of observed vs. modeled heads with both hydraulic conductivity and recharge rate doubled.

Well #	X (m)	Y (m)	I	J	K	Observed head (m)	Simulated head (m)	Error (m)
MW 7	246265	4692177	17	25	1	334.40	335.5	0.65
MW 12	246302	4692217	14	29	1	334.40	335.28	0.88
MW 18	246396	4692151	20	39	1	335.50	335.92	0.42
MW 101	246433	4692151	20	41	1	335.40	336.15	0.75
MW 103	246373	4692101	26	37	1	335.00	335.83	0.83
MW 105	246265	4692128	23	25	1	334.60	335.11	0.51
MW 106	246348	4692179	17	31	1	335.00	335.59	0.59
MW 112	246299	4692178	17	29	1	334.40	335.26	0.86
MW 113	246255	4692128	23	24	1	334.50	335.05	0.55
MW 115	246396	4692136	22	39	1	335.60	335.93	0.33
MW 118	246337	4692178	17	33	1	335.10	335.52	0.42
Root Mean Square Error = 0.64								

A.5 Contaminant Transport Modeling

The contaminants of concern are benzene and xylene released from LUST site 8LTU14 (the red triangle in Figure A-1). The benzene plume and xylene plume are simulated with MT3DMS in GMS v. 3.1 based on the steady-state groundwater flow condition obtained in Section A.4.

A.5.1 Model Conceptualization and Design

The simulation domain for contaminate transport is the same as that for groundwater flow shown in Figure A-1, with no solute flux across any boundary. The LUST site is treated as an internal constant concentration source with benzene at 14,000 ppb and xylene at 6200 ppb (Table

A-7). These concentrations are the highest reported for the two hydrocarbons from monitor well samples at the source LUST site (8LTU14). The constant source condition represents a conservative scenario even though the times and amounts of petroleum releases from the sources are uncertain.

Table A-7. Source locations and concentrations at the LUST site 8LTU14.

LUST #	X (<i>m</i>)	Y (<i>m</i>)	I	J	K	Benzene Concentration (<i>ppb</i>)	Xylene Concentration (<i>ppb</i>)
8LTU14	246395	4692151	20	39	1	14,000	6,200

A.5.2 Input Parameters

Four packages, Basic, Advection, Dispersion, and Chemical Reactions, are used in MT3DMS. Some of the parameters in the Basic package are listed in Table A-8. One stress period of 3650 days is used. The method of characteristics (MOC) is selected in the Advection package.

Table A-8. Stress period and time step information in Basic package of MT3DMS

Stress period	Stress period length (<i>day</i>)	Max transport steps	Initial time step size	Time step bias	Max time step size
1	3650	20000	365	1	365

The other parameters needed in this simulation are effective porosity (n_e), dispersivity (α), adsorption constant (K_d), and biodegradation rate (λ). These parameters have not been determined from aquifer samples, so assumptions were made based on available data and the

borehole log descriptions. The value for effective porosity is estimated to be 0.2. The value for longitudinal dispersivity (α_x) is estimated based on the minimum plume length (between 8LTR14 and the farthest contaminated monitor well (EnecoTech, 2000) of about 700 ft. The estimation formula of Neuman (1990) yields a value of 73 ft (22 m). However, a value of 15 m is used for α_x because part of large-scale heterogeneity (i.e., layering) that contributes to dispersion has been considered explicitly. Horizontal and vertical transverse dispersivity (α_y) were taken as 0.75 m, and molecular diffusion was neglected since it is much smaller than pore-scale mechanical and macro-dispersion. Uncertainty in dispersivity is addressed in the sensitivity analyses. The distribution coefficient for benzene is $0.081 \text{ cm}^3/\text{g}$ and that for xylene is $0.177 \text{ cm}^3/\text{g}$. These values for K_d were selected to give retardation factors of 1.5 for benzene, and 4.5 for xylene, consistent with behaviors of these compounds in field studies (Wiedemeier et al, 1995). The biodegradation rate was set as 0.0001 day^{-1} for both layers and both contaminants. The values of these parameters are listed in Table A-9.

A.5.3 Model Calibration

A calibration effort in this case would involve systematically adjusting the values of effective porosity (n_e), dispersivities (α_L , α_T), biodegradation rate (λ), and distribution coefficients (K_d) in successive simulations, and comparing the results against the observed concentration at the monitoring wells. The transport model has not been fully calibrated. As the model now stands, the gross plume shapes from the simulations can be compared with mapped contamination from the field data.

Table A-9 Input parameters for contaminant transport modeling

	Layer 1	Layer 2
Effective Porosity, n_e	0.2	0.2
Longitudinal Dispersivity, $\alpha_L (m)$	15	15
Transverse Dispersivity, $\alpha_T (m)$	0.75	0.75
Biodegradation Rate, $\lambda (day^{-1})$	0.0001	0.0001
Bulk density (g/cm^3)	1.86	1.86
Distribution coefficient, $K_d (cm^3/g)$ for Benzene	0.081	0.081
Distribution coefficient, $K_d (cm^3/g)$ for Xylene	0.177	0.177

Figure A-5a illustrates the benzene plume in both layers after 10 years using the parameters listed in Table A-9. Figure A-5b is a close view of the benzene plume shown in Figure A-5a. Figure A-6a is the comparable xylene plume and Figure A-6b is a close view of Figure A-6a. The maximum length and width of the modeled benzene plume in the two layers are listed in Table A-10. The plume boundary is set at the concentration of 100 ppb due to the accuracy of the numerical scheme used in the MT3DMS. It is seen that both the length and width of the plume increase much faster at earlier years than later years and the plume, especially its width, became almost stable after seven or eight years. Actual site monitoring data show that neither benzene nor xylene have ever been detected in the loess layer as far downgradient as MW-7. Nor have they been detected in MW-114 (not listed, located south of MW-113), which provides a constraint on plume spreading. Benzene but not xylene has been detected in residential wells #4 and #11, indicating the contaminant plumes have entered the sand layer down gradient from the source. The lack of contaminant detection in well #6 is a constraint on plume spreading in the sand layer. With a calibrated model, evolution of the

benzene and xylene plumes could be simulated with greater confidence, and predictions about plume behavior could be made.

Table A-10 The length and width of the benzene plume at different times

Time (year)	Layer 1		Layer 2	
	Length	Width	Length	Width
1	125	45	144	55
2	168	55	172	66
3	185	71	188	71
4	186	74	201	73
5	205	78	207	78
6	216	85	226	84
7	228	88	232	90
8	236	92	244	91
9	244	92	252	92
10	252	92	258	92

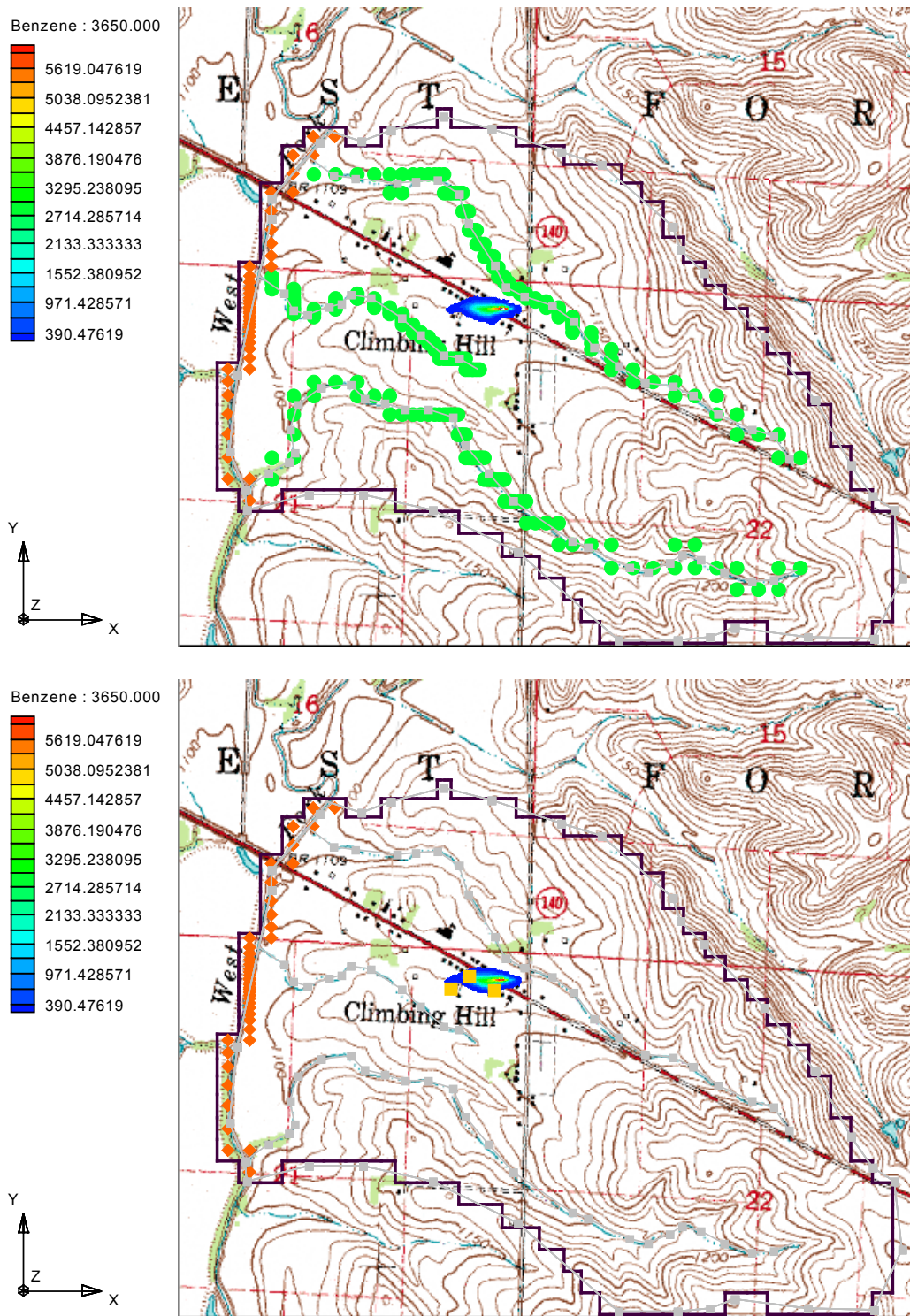


Figure A-5b Benzene concentrations at 3650 days in layer 1 (top) and in layer 2 (bottom)

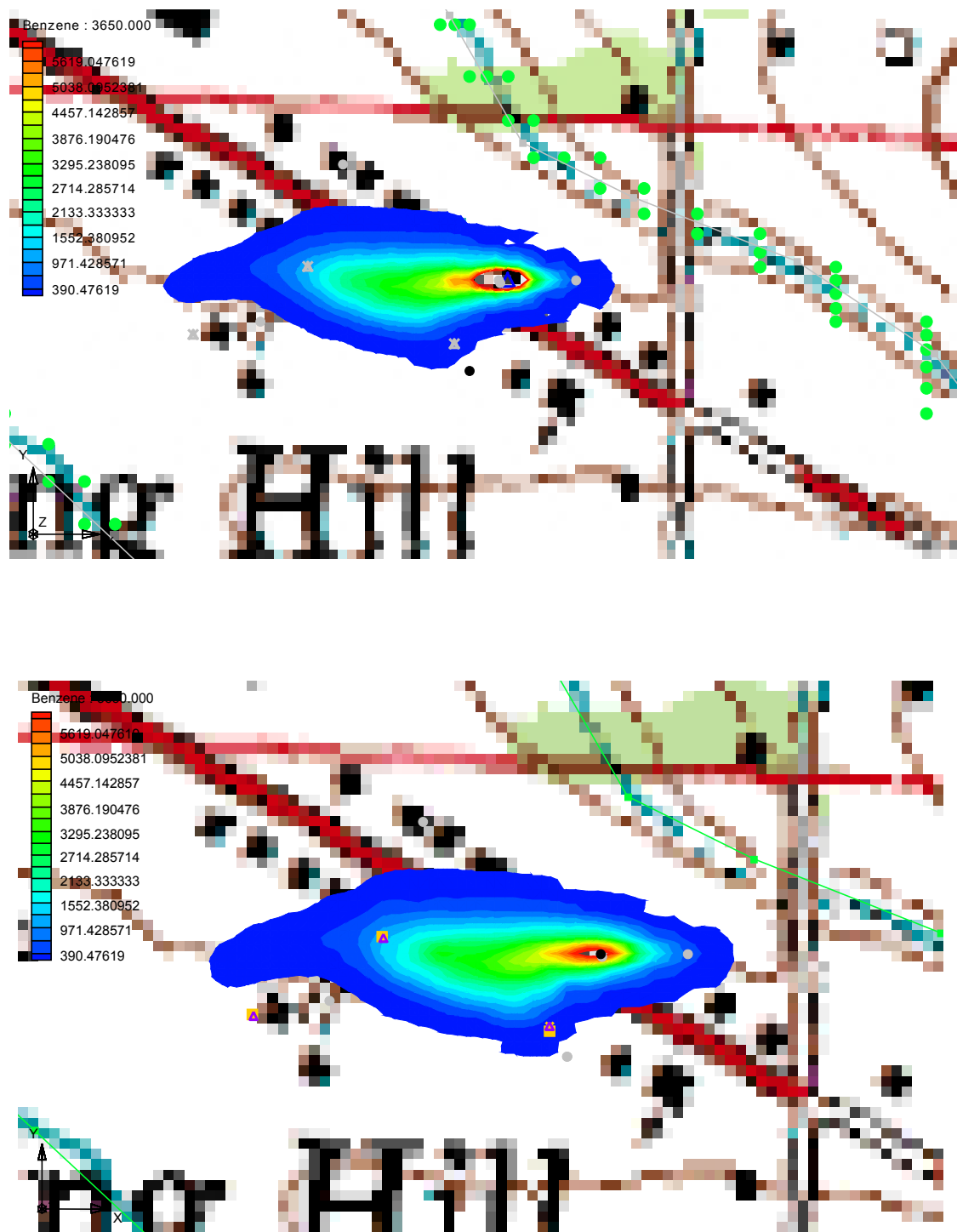


Figure A-5b Close view of Benzene concentrations at 3650 days in layer 1 (top) and in layer 2 (bottom)

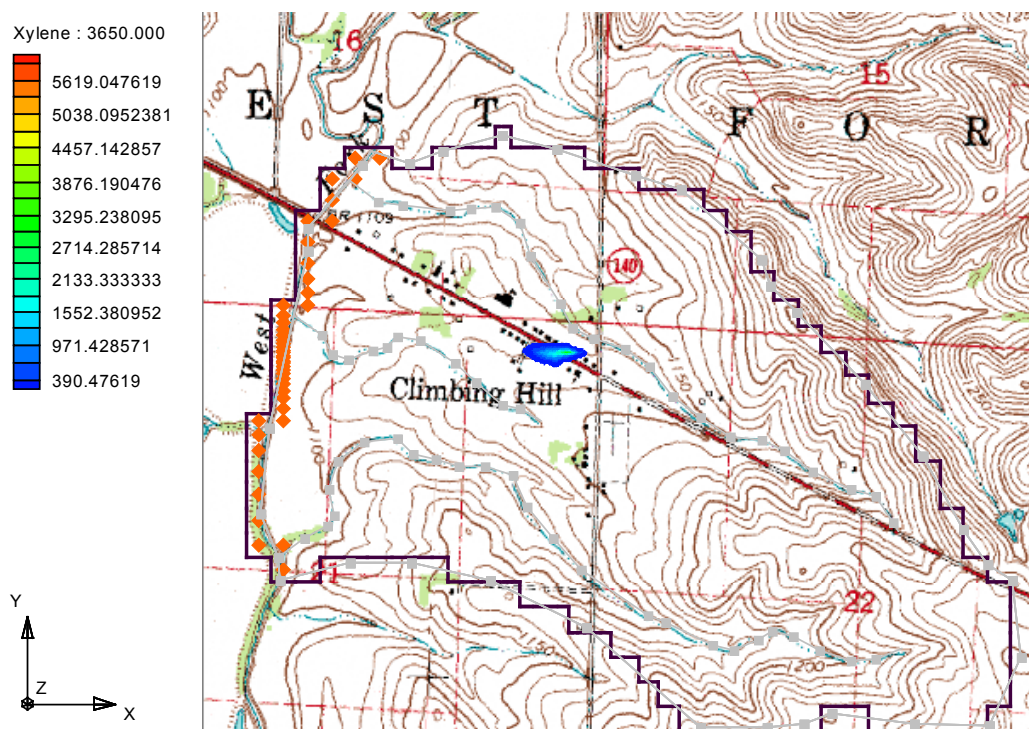
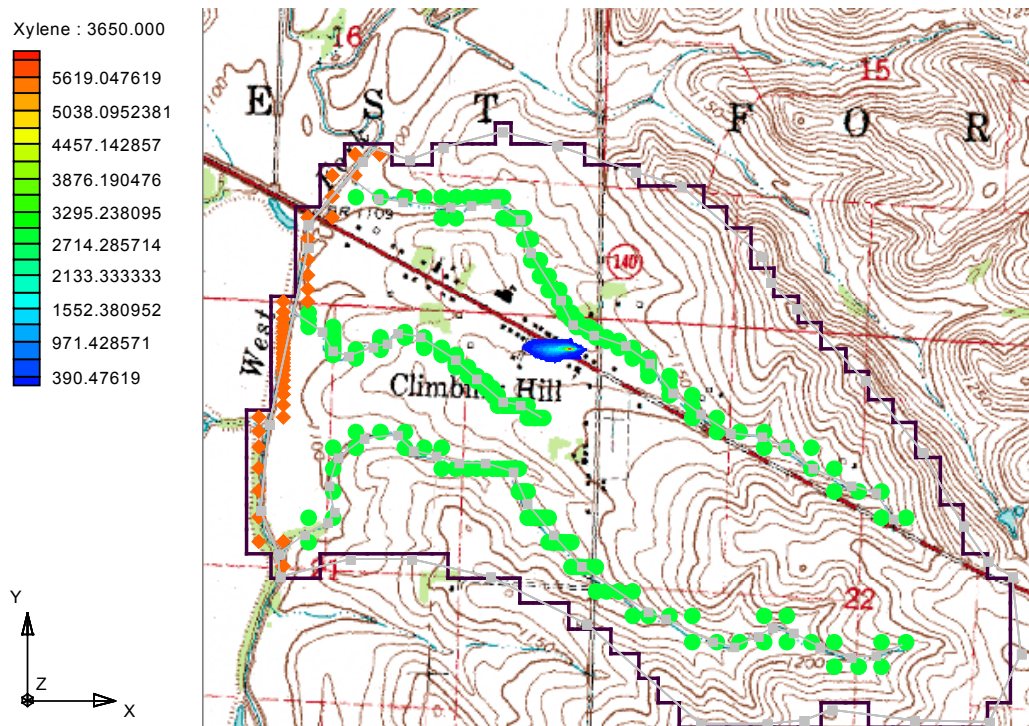


Figure A-6a Xylene concentrations at 3650 days in layer 1 (top) and in layer 2 (bottom)

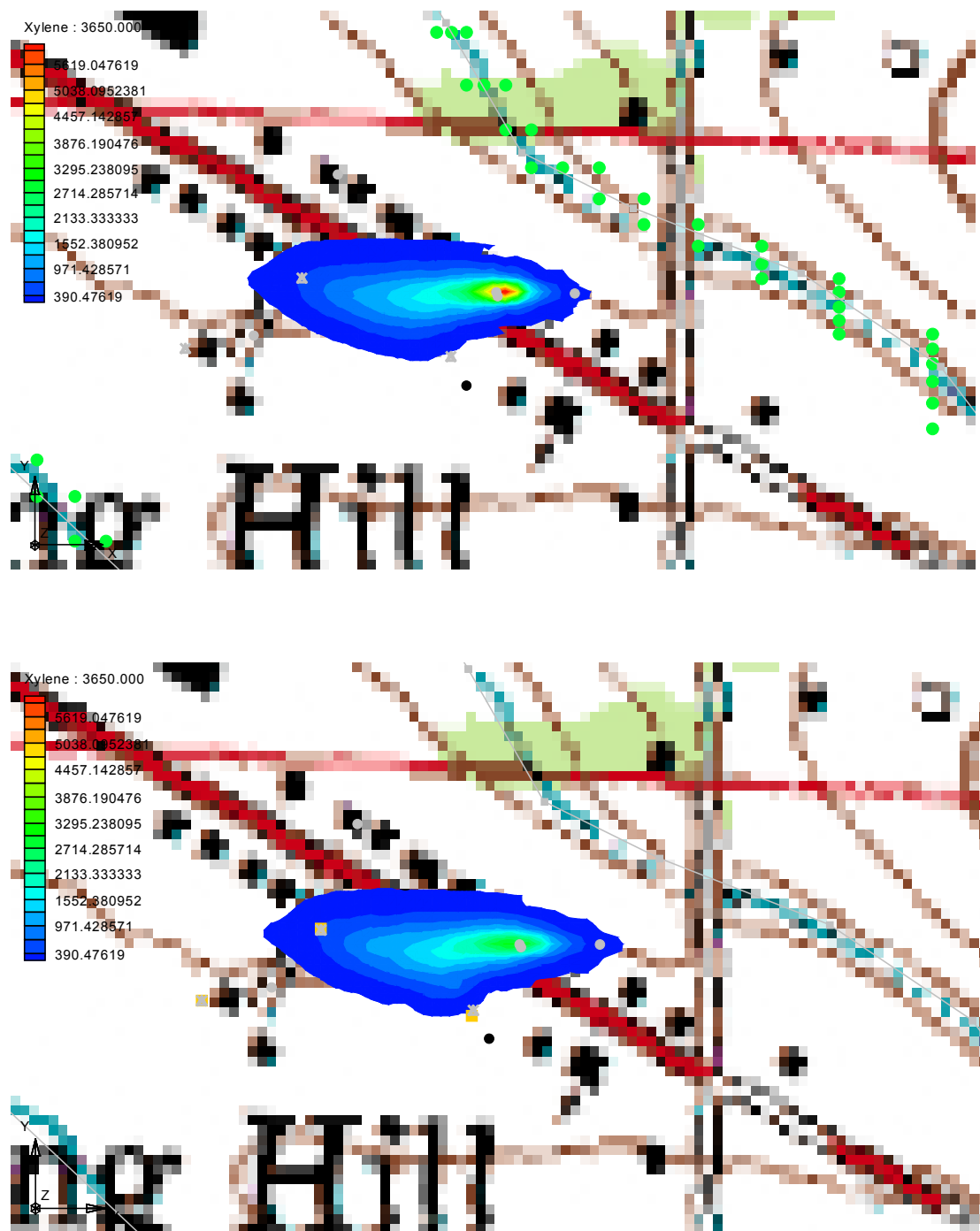


Figure A-6b Close view of xylene concentrations at 3650 days in layer 1 (top) and in layer 2 (bottom)

A.6 Summary and Conclusions

Calibrated results of the flow model indicate hydraulic conductivities chosen for the two layers are reasonable. The recharge value is within the reasonable range for western Iowa. Groundwater flow direction is westward through Climbing Hill in the shallower aquifer. Low capacity residential water wells have little effect on the local groundwater gradient. The location of many of these wells is in the direct, down-gradient position from the contamination source. This fact was the main condition responsible for contamination reaching the water wells. The shale layer separating the shallow, contaminated water source from an underlying sand in the upper portion of the Dakota Fm. appears to be an effective protection of the Dakota Fm.

The stratigraphic configuration of a higher permeability layer beneath a lower permeability layer, together with water wells pumping from the higher permeability layer, creates a condition for vertical flow from the water table toward the underlying layer. Petroleum constituents dissolved in groundwater will be transported downward from the water table into the higher permeability layer. The transport model needs to be further calibrated and its sensitivity to the parameter changes needed to be explored, although initial modeling of the benzene and xylene plume seem to be agree reasonably with observed concentration. If biodegradation is not a discriminating nor particularly influential parameter, benzene can reasonably be expected to migrate at three times the rate of xylene, suggesting that releases of heavier products than gasoline will be strongly retarded.